Pentyl 2-hydroxypropanoate

6382-06-5	DTXSID70858752

Model Performance

Mode	Data

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.85	0.69	0.86	0.67	0.86	0.78	

Model Results

Predicted value: 1.60

Global applicability domain: Inside

Local applicability domain index: 5.94e-01

Confidence level: 7.04e-01

Nearest Neighbors from the Training Set

Image not found

Methyl pivalate Measured: 1.83 Predicted: 1.76 Image not found

Butanoic acid, 3-methyl-, methyl

ester

Measured: 1.82 Predicted: 1.83 Image not found

Methyl valerate Measured: 1.96 Predicted: 1.84

Image not found

Ethanol, 2-(1,1-dimethylethoxy)-

Measured: 0.39 Predicted: 6.54e-01 Image not found

Isobutyl acetate
Measured: 1.78
Predicted: 1.82